SimDOME

# User Story: A detailed stochastic investigation on morphology and fractal dimension of carbon black aggregates

**Aims**

- To predict the evolution of fractal dimension of carbon black aggregates along the length of the reactor

**Methodology**

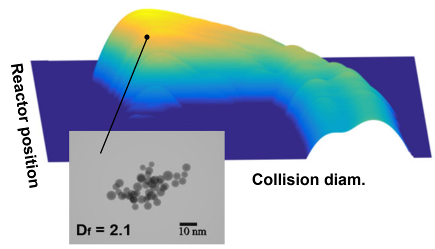
- Develop Population Balance Models for particles
- Combine with detailed kinetics models in a PFR

**Results**

- Carbon Black's evolution of Particle Size Distribution
- Fractal dimension of the sampled aggregates

## Summary


Carbon Black (CB) is a nano-sized material of the form of colloidal particles that are produced by incomplete combustion or thermal decomposition of gaseous or liquid hydrocarbons. Some of the CB applications are tyre, rubber, plastic or coating industries where specific particle size distribution (PSD), surface area or even morphology of produced particles are required. This example describes how morphology of CB particles, in form of 3D structures of CB aggregates and their fractal dimensions, can be calculated using CMCL's *k*inetics™ software.


## Case Description

An experimental scenario has been selected from literature [1], where CB aggregates were synthesised in a heated tubular reactor via thermal pyrolysis of various mixtures of benzene and acetylene in nitrogen. The selected scenario is schematically shown on Fig.1. The Carbon Black system model formulated within *k*inetics™ comprises a detailed gas-phase chemical kinetic model and a detailed particle-phase stochastic population balance model.

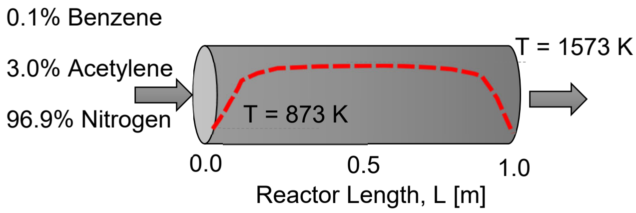



Figure 1: Process conditions selected from the literature [1]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## Morphology And Fractal Dimension Prediction

Upon successful solution of the CB system, detailed information about a number of representative aggregates (number and size of primaries, chemical composition, collision diameter etc.), selected at specified reactor's positions is then used to create 3D structures (in the form of a TEM-like image) of the sampled aggregates via ballistic aggregation procedure.

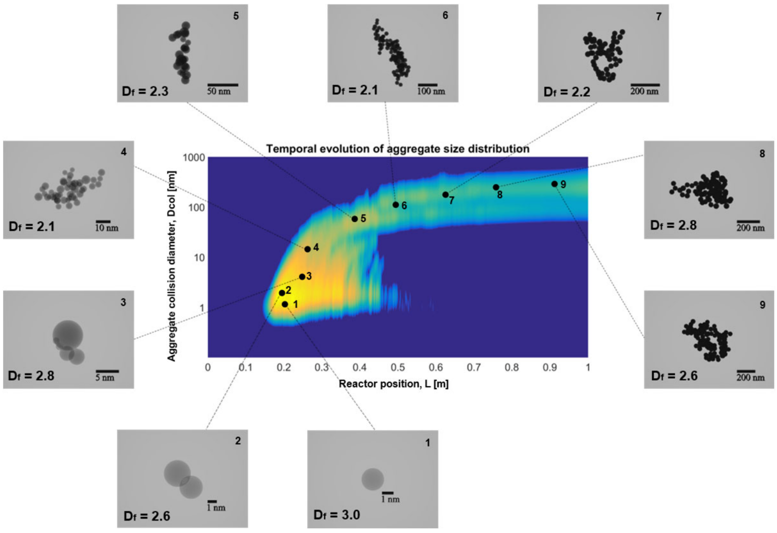


Figure 2: Carbon Black aggregate particle size distribution (PSD) evolution along the reactor.

## Results

Main simulation results in Fig.2 depict the evolution of particle size distribution of carbon black aggregates along the reactor together with calculated morphologies and fractal dimensions of selected aggregates. Colormap encodes normalized particle concentration, dN/dlogD [#/cm3], y axis represents average aggregate collision diameter, Dcol [nm], and x axis shows position on the reactor, L [m].

It can be seen that the CB particles start to form around 0.2m from the reactor's inlet, where the temperature rises to around 1530 K. Initially, the aggregates formed contain small number of primaries and are of spherical shape (1-3), hence their fractal dimension is close to 3.0. Further along the reactor, the aggregates start to coagulate and grow via surface reactions. The interplay between these two processes together with constant inception of small primaries leads to the formation of more complex structures (4-7). At the reactor's outlet, the sampled aggregates (8-9) are close to the spherical shape.

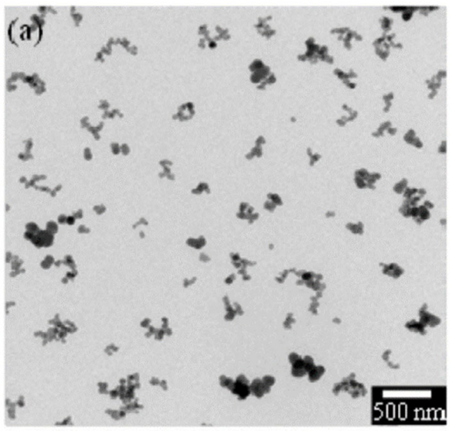


Figure 3: Experimental TEM data from Ono et al. [1].

Comparing sampled aggregates with the experimental TEM image from the literature [1] shows that there is an agreement in terms of morphology and aggregate sizes.

The development achieved via the SimDOME project helps in better understanding of morphology and details of Carbon Black production in industry. SimDOME project's partner CMCL intend to exploit these results via further uptake of its toolkit *k*inetics™ to solve these industrial problems.

## References


[1] K. Ono, M. Yanaka, Y. Saito, H. Aoki, O. Fukuda, T. Aoki and T. Yamaguchi, Chem. Eng. J., 215-216, 2013.



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